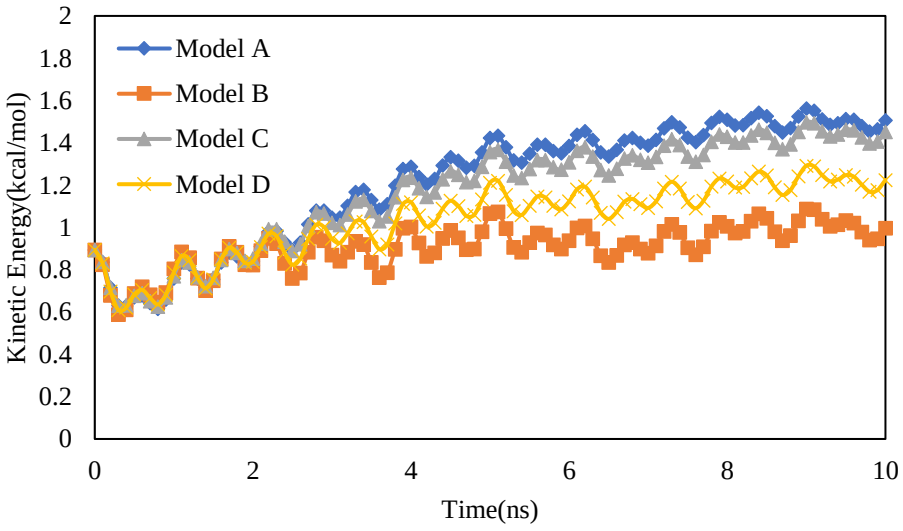
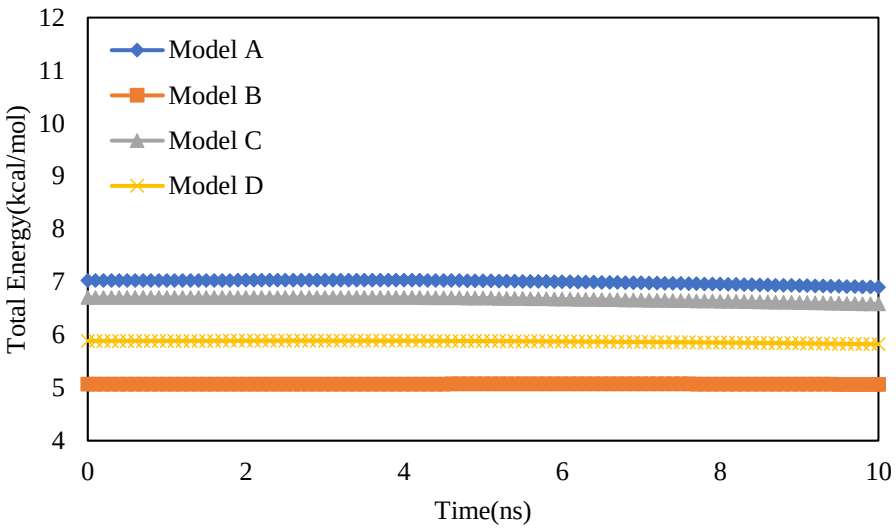
Supplementary

To more computational analysis of atomic stability of modeled samples, the total energy of defined structures reported in Figure 1s. This calculation indicated the total energy value converged to 6.90, 5.06, 5.58, and 5.82 kcal/mol after 10 ns in presence of adiponectin, ghrelin, leptin, and neuropeptide Y hormones receptors, respectively. Physically, the total energy convergence shows the attraction force exist between various particles. This condition caused the atomic collision intensity don't diverge and total system reach to equilibrium phase. Technically, this behavior arises from appropriate MD settings as reported previous computational researches [38-40]. Furthermore, to ensure about simulation time in equilibrium phase of modeled samples, the MD time increased to 100 ns. The total energy outputs for total energy of each systems presented in Table 1s. As shown in this table, the total energy of models A, B, C, and D converged to 6.89, 5.03, 5.56, and 5.84 (respectively) after 100 ns. These numerical values don't appreciably changes rather to 10 ns outputs. So, this comparison indicated the 100 ns is sufficient time to equilibrium phase detection inside computational box. Physically, this performance arises from atomic amplitude resonance convergence to constant value after 10 ns.



(a)



(b)

Figure 1s. (a) Kinetic and (b) total energy changes of various atomic systems in current research as a function of MD time.

Table 1s The total energy outputs of various modeled Biosystems in various MD times.

System ID	After 10 ns (kcal/mol)	After 50 ns (kcal/mol)	After 100 ns (kcal/mol)
A	6.90 ± 0.08	6.92 ± 0.01	6.89 ± 0.05
B	5.06 ± 0.03	5.11 ± 0.02	5.03 ± 0.06
C	5.58 ± 0.06	5.59 ± 0.01	5.56 ± 0.01
D	5.82 ± 0.04	5.80 ± 0.03	5.84 ± 0.04

The validation of these settings and used approach is another important parameter for numerical researches. For this, radial distribution function of O-O molecules inside aqueous environment calculated. The radial distribution function represented the atomic arrangement of target system which can be compared with previous reports. Figure 2s presented output for radial distribution function of O-O molecules inside computational box. This results consistent with previous reports and validated our computational method in our research [41].

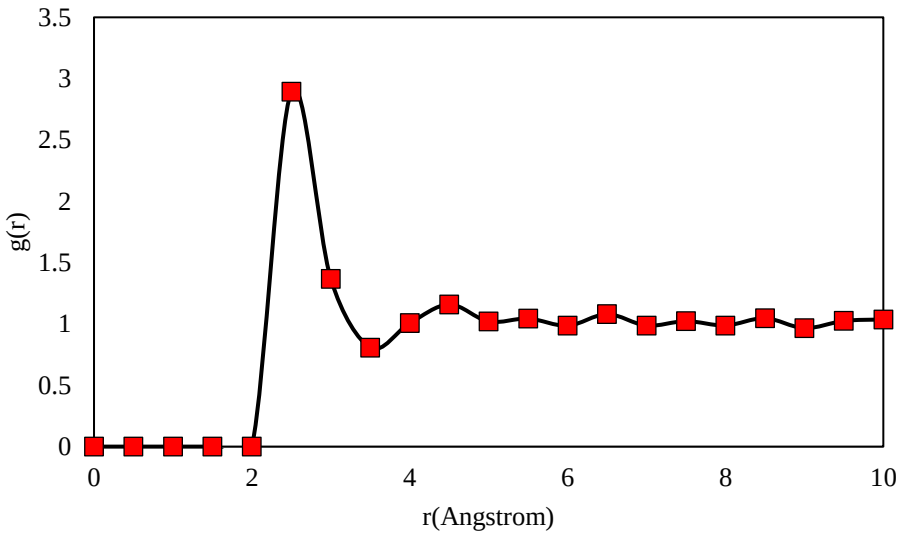


Figure 2s. The radial distribution function of O-O molecules in modeled aqueous environment.